**Many-Body Harmonic Oscillators**

**Quantization of Crystal Lattice**

Might want to see Classical Mechanics folder on lattice oscillations too, for another, more extensive perspective. I’ll be borrowing a lot from those files. We start by considering the Hamiltonian for a set of N atoms, each of mass M. Let the position of the jth atom be **r**j = **R**j + **x**j where **R**j­ is its equilibrium position and **x**j­ is the deviation from equilibrium. The {**R**j} forms a complete basis provided that we assume periodic boundary conditions.

Each of the atoms forms covalent bond or something with its neighbor, making the entire lattice cohesive. The actual potential between the atoms is probably pretty hard to figure out. If we’re dealing with a metal, then we might be able postulate that each of the atoms contributes one or two electrons to the conduction band, and so is left with a +|e| or +2|e| ionic charge. And so each atom exerts an ionic Coulomb force on every other. But for semiconductors or insulators, this doesn’t happen, and so the interatomic force is a little more nebulous. But in any event, it obviously creates a well in the neighborhood of each atom. Let V({**r**m}) be the total potential energy of all the ions (I guess I’m going to call them ions just for sake of discussion) together as a function of their positions. We can expand the potential in a Taylor series about the atoms’ equilibrium positions **r**j = **R**j.



where i = 1…N, j = 1…N, k = 1…N each label the ion, and α = x,y,z, β = x,y,z, δ = x,y,z each denote the components of the respective vector in the x, y, z directions. A more concise way to write this might be:



where the **:** indicates a generalized dot product between tensors. Either way, the first term is a neglectable constant. By presumption, the particles are in a stable potential minimum, experiencing no net force at equilibrium, so the second term is zero. We keep the third term, but neglect the fourth, and all others, for simplicity [well also presuming the deviations from equilibrium are small enough that these terms don’t matter appreciably]. So we’ll define the spring constant tensor which gives the ‘spring constant’ between the two ions located at **R**i and **R**j:



where **e**α and **e**β are the unit vectors in the respective x,y,z directions. And we’ll write the displacement of the ith ion as,



where again α refers to the x,y,z component. So then we have, for our potential:



Note **I** is not a unit vector – it’s a vector displacement (operator). See the Properties of the K Matrix file for argument that we can take Kαβ(Ri,Rj) to be symmetric in α, β, and for Ri and Rj to only enter in the combination ΔRij = |**R**i – **R**j|. And also, implicitly, that due to periodic boundary conditions, the set of {ΔRij} for i fixed, and j running over all ions from 1…N, does not depend on i. Given the statements above, we may write:



So then our total Hamiltonian would be:



We can rewrite this as:



where **x**(**R**) and **p**(**R**) denote the displacement and momentum of the oscillator at position **R**, and satisfy,



To find the eigenstates of H we make the canonical substitutions (suppressing the Greek index for now)



Note that periodic boundary conditions restrict the q’s to N distinct values. For instance, if we’re dealing with a paralleliped with side lengths Lx­ = Nxax, Ly = Nyay, Lz = Nzaz (where ai are the lattice spacings), then periodic boundary conditions require:



We’ll choose the Ni distinct values of qi to be:



We can invert the ‘transform’ to get:



Note that the Hermiticity of xR and pR imply:



This is a canonical transformation so we also have, as one can verify:



Now plug this substitution into H:



Define:



and we can write:



(see Properties of the K Matrix file) So for fixed q, Kαβ(q) is a real symmetric matrix with non-negative eigenvalues that we denote MionΩqλ2, and real eigenvectors **ε**qλ. Now we also have: Kαβ(q) = Kαβ(-q), and so can expect that a similar relationship holds for the eigenvalues:

Ω**q**λ = Ω-**q**,λ. And also for the eigenvectors. But, we can also make the following actually more convenient choice,



which admits the possibility **ε**qλ = **q**, which is useful for longitudinal vibrations and isotropic crystals. Now make an eigenvector expansion (with a certain prefactor choice to keep things canonical):



Then we still have canonically conjugate variables,



and our H comes to:



Finally, we can diagonalize H by defining,



which satisfy bosonic commutation relations, as we can verify,



Solving for x and p we get:



And filling these in we get:



And then finally we have,



Thus the excitation spectrum of the harmonic lattice can be described as a set of non-interacting bosonic excitations or phonons, having energies Ωqλ created and destroyed by aqλ†,

aqλ respectively. If need be, we can recover the ionic displacements and momenta as



and:



Can also rewrite these using ρion = MionN/V. We have implicitly assumed that the lattice has one ion per unit cell. If there are Nb ions in the basis, then there will be 3Nb phonon branches which we can label λ = 1, 2, …., 3Nb. So we have the same frequency spectrum as in the classical case. Each oscillation frequency can have n phonons in it, for an energy of (n+1/2)ωk.

*\* I’ll call the results we have for x(R) and p(R) to be the one’s using the CMT phase convention (see QFT folder/photon quantization too).*

**Phonon Frequencies**

So ion lattices have 3 acoustic modes and 3(p-1) optical modes, where p is the # of atoms in the basis. In an isotropic system, 2 acoustic modes will be perpendicular and 1 will be parallel to q. For a non-spherical Fermi surface, the directions of the vectors would be different. Apropos the frequencies, we need to specify explicitly the form of the ion potential Vii(r). If we presume a long range interaction whereby K(Ri,Rj) is appreciably non-zero for ions separated by a large distance |**R**i – **R**j|, like would be the case if it were to stem from a pair-wise Coulomb repulsion



where Ze is the charge of one ion, then due to the long range character of V(**r**m), the ion gas can support longitudinal plasma oscillations at a frequency that in the long wavelength limit is:

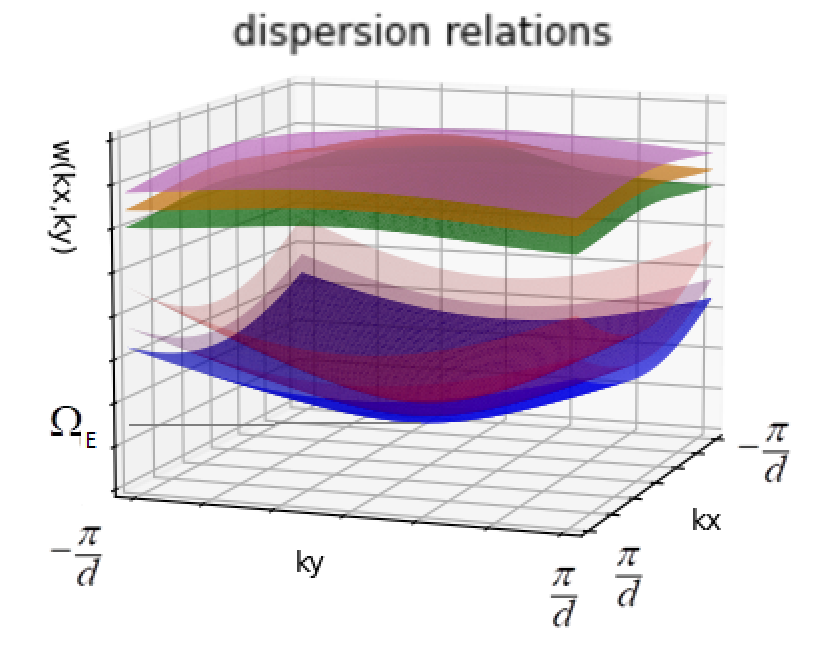


(recall this is the same frequency that we encountered in the Electrodynamics folder). Just to make connection with the plasma frequency, if we had e-‘s in the picture, then overall charge neutrality would require.



So the ionic ‘plasma’ frequency is much smaller than the electronic one, owing mainly to the greater inertia. So it seems our frequency spectrum for the ‘acoustic’ modes would be ‘optical like’, meaning they wouldn’t go to zero as k → 0, but would rather go to ΩE. Can check out the Thermodynamics/Plasma file for an idea of what the entire spectrum would look like; it seems it’d be ~ Ωac(k) = √(ΩE2 + ck2). The reason that Ωac(q) doesn’t go to 0 in this case is because the potential between the particles in the lattice sites is long range, not short range, unlike in the toy problems in previous files. There we do literally assume only n.n. interactions since it is a HO and only adjacent HO’s can interact with each other. Finally, it makes sense that we should have long range modes because if we have a set of atoms bound to lattice sites, we can make them oscillate back and forth in unison with wavelength ∞ if they stay connected to each other, which they will b/c of the long range interaction. This sort of situation would be satisfied if we were in an insulator, or semi-conductor perhaps.

The 3(p-1) optical modes will always have a non-zero minimum regardless of whether the interaction between the ions is short ranged or long ranged, and be higher frequency than the acoustic modes I think. These are the oscillation frequencies of molecule that makes up the basis, basically. For p = 2, altogether we’d get something like this:



But if we have short ranged interactions between bases (as would happen in a metal where the conduction electrons could screen the ion-ion interaction, thereby exponentially damping it), then the acoustic spectrum drops to zero at the origin, and we get something like this below, for p = 2 atoms in the basis. Note the ‘optical’ part of the spectrum won’t really be affected either way.

Chart, surface chart

Description automatically generated

And last,

**Wavefunctions**

I guess I’ll just write down what the wavefunction ought to be, without actually being too rigorous. Can check the last file for more information. But let’s say we start from,



where,



Let’s put H in position space, of sorts. We can write,



Now x-q,λ = xq,λ\*, so we can write this as:



[this is what I did in previous file, but need to think more about this] And we can change variables to Xkλ = Re(xkλ), Ykλ = Im(xkλ). Then as in previous file, we’ll find:



And then since Yq,λ = X-q,λ, can extend the sum to both sides of the BZ and say,



And it follows that our wavefunction is:



where,



and **x**R is the coordinate of the **R**th oscillator. Hn are the Hermite polynomials of course. And for completeness, I’ll just add:



So this wavefunction would have N 3d coordinates, so 3N independent variables. Not exactly something you’d want to do a lot of calculating with. So this is why we use the creation/annihilation operator formalism when dealing with these states. And likewise with the 2nd quantization formalism when dealing with many-body identical particle states.